Researchers find potential key for unlocking biomass energy

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LANL molecular model helps expose cellulose weakness

LOS ALAMOS, New Mexico, July 20, 2011—Researchers at the U.S. Department of Energy's Los Alamos National Laboratory and Great Lakes Bioenergy Research Center have found a potential key for unlocking the energy potential from non-edible biomass materials such as corn leaves and stalks, or switch grass.In a paper appearing in today's Journal of the American Chemical Society, Los Alamos researchers S. Gnanakaran, Giovanni Bellesia, and Paul Langan join Shishir Chundawat and Bruce Dale of Michigan State University, and collaborators from the Great Lakes Bioenergy Research Center in describing a potential pretreatment method that can make plant cellulose five times more digestible by enzymes that convert it into ethanol, a useful biofuel.Biomass is a desirable renewable energy source because fermentable sugars within the cellulose network of plant cells can be extracted with enzymes and then converted into ethanol—if only it were so simple. One of the key difficulties in creating biofuels from plant matter is that the cellulose tends to orient itself into a sheet-like network of highly ordered, densely packed molecules. These sheets stack upon themselves and bond together very tightly due to interactions between hydrogen atoms —somewhat like sheets of chicken wire stacked together and secured by loops of bailing wire. This stacking and bonding arrangement prevents enzymes from directly attacking most of the individual cellulose molecules and isolating the sugar chains within them.Currently, ethanol can only be extracted in usable quantities if the biomass is pretreated with costly, potentially toxic chemicals in an energy-intensive process. Now, however, the research team has discovered a way to develop potentially cost-effective pretreatment methods that could make biomass an economically viable contender in the biofuels arena.Using recent experimental data provided by their journal collaborators, Gnanakaran and his Los Alamos colleagues used state-of-the-art computational methods and molecular modeling to examine how cellulose changes structurally into an intermediate form that can be enzymatically attacked when pretreated with ammonia.“Our modeling showed, and the experimental evidence confirmed, that the pretreatment reduced the strength of hydrogen bonds in the cellulosic network,” said Gnanakaran. It was as if the bailing wire in the bound chicken-wire analogy had been removed and replaced more loosely with thread. This, in turn, significantly reduced the tightness of the cellulose network and left it more vulnerable to conversion into sugar by fungi-derived cellulolytic enzymes.The end result is a potentially less costly and less energy intensive pretreatment regimen that makes the cellulose five times easier to attack.“This work helps address some of the potential cost barriers related to using biomass for biofuels,” Gnanakaran said.In addition to LANL, the GLBRC, and Michigan State University, the paper included collaborators from American University and the U.S. Department of Agriculture’s Forest Products Laboratory in Madison, Wisconsin.The LANL work is funded in part by the Laboratory-Directed Research and Development Program. Computing resources used in the research are housed at Los Alamos and provided under LANL institutional computing.